Collective Excitations in InAs Quantum Well Intersubband Transitions

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Abstract

Intersubband transitions in semiconductor quantum wells are studied using a density matrix theory that goes beyond the Hartree-Fock approximation by including the full second order electron-electron scattering terms in the polarization equation for the first time. Even though the spectral features remain qualitatively similar to the results obtained with the dephasing rate approximation, significant quantitative changes result from such a more detailed treatment of dephasing. More specifically, we show how the interplay of the two fundamental collective excitations, the Fermi-edge singularity and the intersubband plasmon, leads to significant changes in lineshape as the electron density varies.

Key words: Many-body effects, intersubband transitions, carrier scattering, Fermi edge singularity, intersubband plasmon
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1 Introduction

Intersubband transitions are the underpinning physical mechanisms for quantum cascade lasers (QCLs) and quantum well infrared photodetectors (QWIPs). Detailed understanding of the transition processes has to include the spectral features of intersubband absorption. From a technological perspective, such understanding will allow better QCL and QWIP design and optimization. At the same time, spectral features also involve many issues that are of importance to fundamental physics, such as many-body effects and dephasing of optical polarizations due to electron scattering.

In the past, attention has been paid to the spectral peak position in the intersubband transitions and the related many-body effects. The issue of many-body effects on lineshape received almost no attention. The most extensively studied many-body effects include intersubband plasma (ISP) oscillation, exchange self-energy (XSE), and the Fermi-edge singularity (FES) [2–16]. The current understanding of many-body effects in ISBRs can be summarized as follows: Using the self-consistent field approach [17], ISBR oscillator strength was shown [3,9] to "collapse" into a sharp collective mode, which is blue-shifted relative to the free-carrier spectrum. This is known as the depolarization effect. In this mean-field approach, collective response of ISP is the *only* contribution. In contrast, both FES and ISP resulting from the Fock and Hartree interaction, respectively, can be modeled on the same footing by directly treating the vertex term. It was shown [10] that inclusion of the vertex term leads to a red shift of the absorption peak from that of the mean-field theory. The spectrum peak is then between the free-carrier peak and the depolarization dominated peak, with the spectral shape being dominated by FES [10].

Recently, we have more systematically studied the intersubband absorption spectrum and the interplay of the two collective excitations (FES and ISP) in intersubband transitions using the intersubband semiconductor Bloch equations (ISBEs) [18]. It was found that such interplay leads to significant lineshape changes. The spectral features can change from being FES-dominated to ISP-dominated as well-width increases. There is, however, one potential weakness of that paper, namely the effects of various dephasing mechanisms are approximated by a decay constant in the polarization equation. Since it is known from interband lineshape theory that detailed scatterings will change the lineshape significantly [19,20], it is natural to ask how such scattering will affect the intersubband lineshape and therefore the results of our earlier paper [18].

This paper is a follow-up to Ref. [18]. We will continue the discussion of the interplay of the FES and ISP and discuss the spectral change as electron density is increased. This will be done first under the dephasing rate approx-

imation. We will then discuss the effect of detailed electron scattering using the extended ISBEs which now includes the full second order scattering terms.

2 Theory

Our approach is based on the density matrix theory [19,21] which describes ISBRs in terms of the intersubband semiconductor-Bloch equations, in analogy to the SBEs for interband transitions [19]. Only two conduction subbands are considered in this work. The ISBEs, derived similarly as for interband SBEs [19,21], are given as follows:

$$\frac{df_{l\boldsymbol{k}}}{dt} = (-1)^l \mathcal{I}m\left(2\Omega_k p_{\boldsymbol{k}}\right) + \left.\frac{df_{l\boldsymbol{k}}}{dt}\right|_{inc}, \tag{1}$$

$$\frac{dp_{\boldsymbol{k}}}{dt} = \frac{1}{i\hbar}(\varepsilon_{2\boldsymbol{k}} - \varepsilon_{1\boldsymbol{k}})p_{\boldsymbol{k}} + i\Omega_k(f_{1\boldsymbol{k}} - f_{2\boldsymbol{k}}) + \left.\frac{dp_{\boldsymbol{k}}}{dt}\right|_{inc}, \tag{2}$$

where $\Omega_k = \left[\boldsymbol{d}_{\boldsymbol{k}} \cdot \boldsymbol{E}_\perp(t) - \varepsilon_{21\boldsymbol{k}}\right]/\hbar$. $f_{l\boldsymbol{k}}$ ($l = 1, 2$ for ground and first excited subbands respectively) and $p_{\boldsymbol{k}}$ are distribution functions and intersubband polarization, respectively. $\boldsymbol{k}$ is the in-plane wavevector. $\mathcal{I}m$ means taking the imaginary part of the argument. The QW plane is normal to the $\hat{\boldsymbol{z}}$ direction. $\boldsymbol{d}_{\boldsymbol{k}}$ is the $\hat{\boldsymbol{z}}$-component of the dipole matrix element. $\varepsilon_{l\boldsymbol{k}} = E^{(0)}_{l\boldsymbol{k}} + \varepsilon_{ll\boldsymbol{k}}$ consists of subband dispersion (first term) and the XSE (second term). Furthermore, the subscript inc in general stands for electron-electron and electron-phonon scatterings [19,21], and possibly other dephasing mechanisms. Under the dephasing rate approximation, this term is given by $dp_{\boldsymbol{k}}/dt|_{inc} = -\gamma_p p_{\boldsymbol{k}}$. In a more detailed treatment of scattering [19,21], successive approximation of higher order correlation beyond the Hartree-Fock approximation leads to the second order scattering of the form:

$$\left.\frac{dp_{\boldsymbol{k}}}{dt}\right|_{inc} = -\sum_{\boldsymbol{k}'} W_{\boldsymbol{k}'\boldsymbol{k}} p_{\boldsymbol{k}} + \sum_{\boldsymbol{k}'} W_{\boldsymbol{k}\boldsymbol{k}'} p_{\boldsymbol{k}'} \tag{3}$$

In this paper, we only consider electron-electron scattering. The scattering matrix $W_{\boldsymbol{k}\boldsymbol{k}'}$ is of the second order in the Coulomb potential. The first term contains scattering process out of the $\boldsymbol{k}$ state to all the other states $\boldsymbol{k}'$, which depends on $\boldsymbol{k}$ only and can be approximated as a $\boldsymbol{k}$-dependent dephasing rate. The second term describes so-called in-scattering from all the other states $\boldsymbol{k}'$ to the $\boldsymbol{k}$ state. It depends on both $\boldsymbol{k}$ and $\boldsymbol{k}'$ and is sometimes called a non-diagonal scattering term. The diagonal and non-diagonal terms have a certain cancellation effect. Such a cancellation effect is quite important in determining the lineshape of interband transitions [19,20] and in the ultrafast carrier dynamics [22], and has been systematically studied in the last few

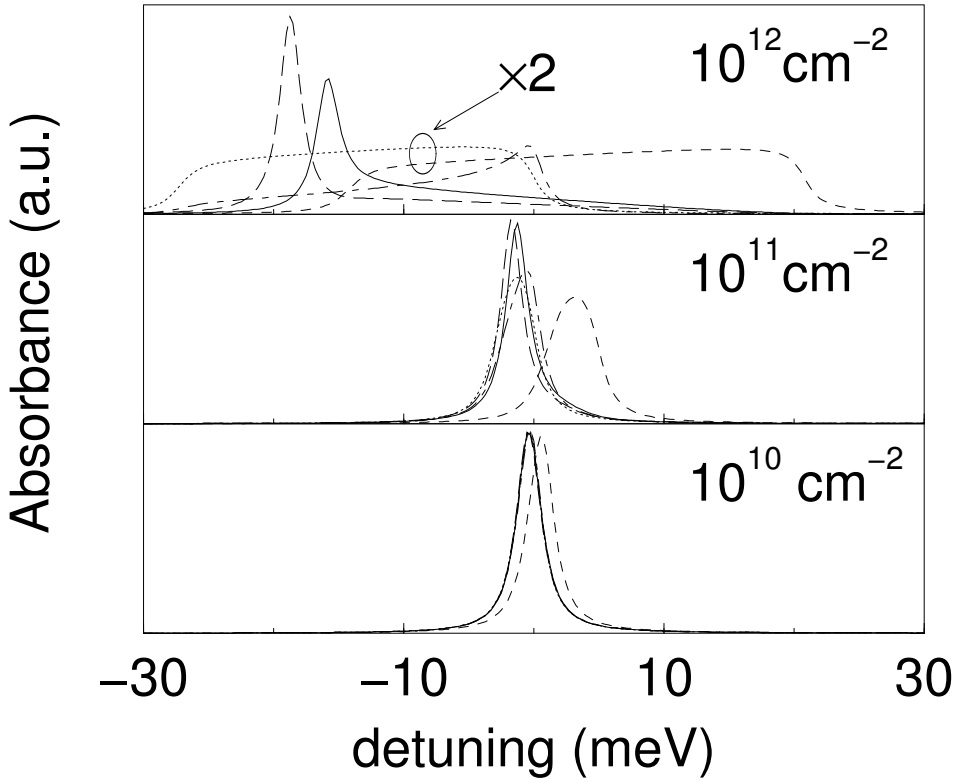

Fig. 1. Intersubband absorbance calculated under the dephasing rate approximation at different electron density levels for a 7nm InAs/AlSb quantum well. The solid curve includes all first order Coulomb interaction terms (full result), as compared with the dotted curve for the free-carrier result. The dashed curve contains XSE, while the long dashed curve contains both XSE and vertex correlation (VTX). The dot-dashed curve contains the depolarization effect. Temperature is at 12K.

years. The effect of this in-scattering term on intersubband transitions has not been reported in the literature.

3 Numerical Results

Fig. 1 shows the intersubband absorption spectra for a 7nm InAs/AlSb quantum well at three different levels of electron density. At each density, we compare absorption spectra with some of the individual many-body effects kept while others are artificially ignored to isolate and identify individual effects. The five curves with different line styles represent five cases: free carrier (dotted), XSE (dashed), exchange interaction including both XSE and vertex term (long-dashed), depolarization effect (dash-dotted), and full result (solid). At low density as shown by the bottom panel, the Coulomb effect is very week and all other curves are indistinguishable, except the dashed curve which includes the XSE. But the curve with the full many-body effects still overlaps

with the free-carrier result. As density increases (see middle panel), the XSE effect becomes more pronounced and the dashed curve moves further away from the rest of the curves. At the same time, the difference among all the other curves also increases as compared to the bottom panel.

At high density levels (top panel), various many-body effects become important and all of them result in an absorption curve very different from the free-carrier one. The free-carrier absorption curve itself becomes very broad, with a flat top. This is a result of 2D density of states and the degenerate nature of the electron gas at such density. The former leads to a sharp drop of the curve at the high energy end, while the latter to a similar drop at the lower end. The wide spectrum and the flat top are a result of the Pauli exclusion principle. The XSE effect broadens the free-carrier curve slightly and mainly moves this curve further up to a higher energy range. This is due to the reduction in energy of the heavily populated ground subband, while the almost empty first excited subband is unchanged. Inclusion of the depolarization effect leads to a somewhat narrowed, but largely distorted absorption spectrum without much blue-shifting as indicated by the dot-dashed curve. The depolarization effect is a result of excitation of intersubband plasmon, a collective excitation in intersubband optics. The effect of the vertex term is remarkable. Its inclusion in addition to the XSE leads to a significant narrowing and downward shifting of the spectrum indicated by the long dashed curve. This feature is closely related to the Fermi edge singularity and it indicates an important collective excitation due to the strong correlation of the degenerate electrons. Finally, the solid line represents the effects of all the first order Coulomb terms that we consider here. This curve, clearly, bears no resemblance to the free-carrier result. The absorption spectrum is completely dominated by the many-body effects. Furthermore, the solid curve is quite close to the long dashed curve, which shows strong features of the FES. What we see here is a competition or interplay of two collective excitations, the FES and the ISP. The relative strength of the two depends strongly on other parameters such as electron density and QW width [18]. For the relatively narrow QW of 7nm in width, the ISP is quite weak, while the FES is the dominating excitation. As a result, the full result (solid curve) is very close to the result with the exchange interaction only.

The result of such an interplay changes as we increase the well width. An example of this situation is shown in Fig. 2 where a wider QW of 20nm in width is considered for three density levels. The spectra at low density levels represented in the bottom and middle panels show similar behavior to that of Fig. 1. The top panel shows spectral features that are significantly different from the case of the narrow well shown in Fig. 1. First, the spectrum with depolarization effect included (dot-dashed line) shows a much narrower and largely enhanced peak, which is blue-shifted compared to the free-carrier spectrum. At the same time, the effect of the exchange interaction represented by

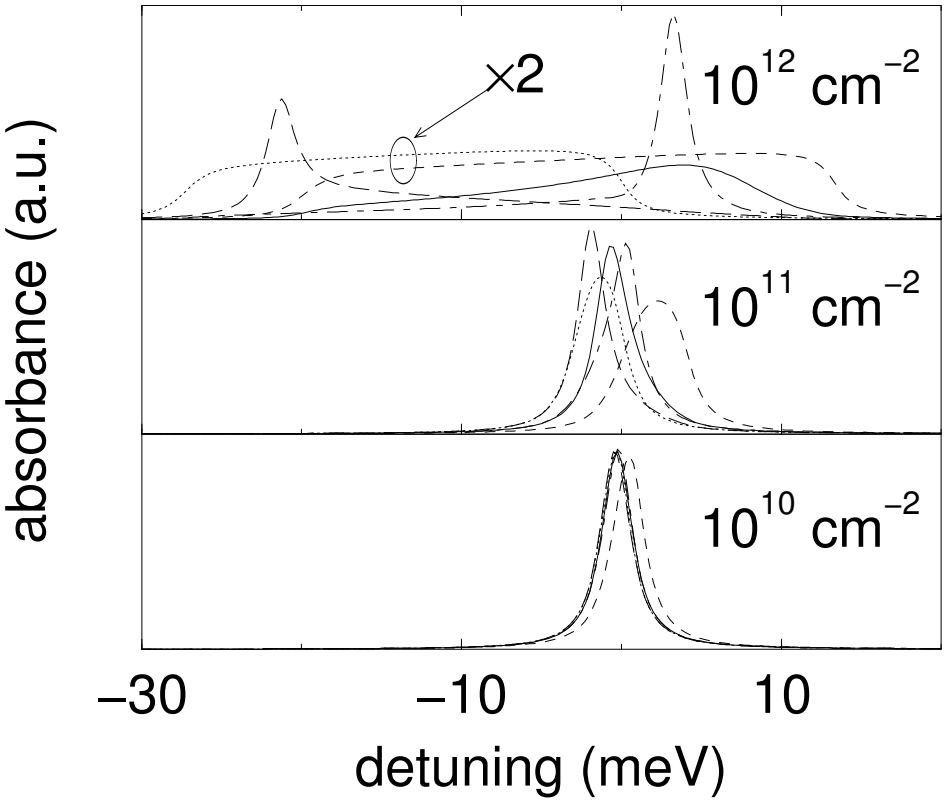

Fig. 2. Same as in Fig. 1 but with a 20nm quantum well.

the long dashed curve is reduced. The ISP is a dominant player in the interplay with the FES-related collective excitation. As a result, the spectrum with the complete first order many-body effects (solid line), more closely resembles the dot-dashed curve with depolarization only. All the results shown so far are obtained under the dephasing rate approximation. To show how a detailed treatment of electron-electron scattering with the complete second order terms will change the situation, we solve the polarization equations now with the full diagonal and off-diagonal scattering terms as given by Eqn. (3). Overall, the results show that the second order scattering will not change the qualitative behavior of the spectrum, but it does change the lineshape and peak absorption values quantitatively. We see that the diagonal scattering term alone gives the smallest peak absorption value and longest tail (see the inset). The inclusion of the off-diagonal scattering has some cancellation effects with the diagonal term. As a result, the peak absorption is the highest and the absorption tails are the shortest.

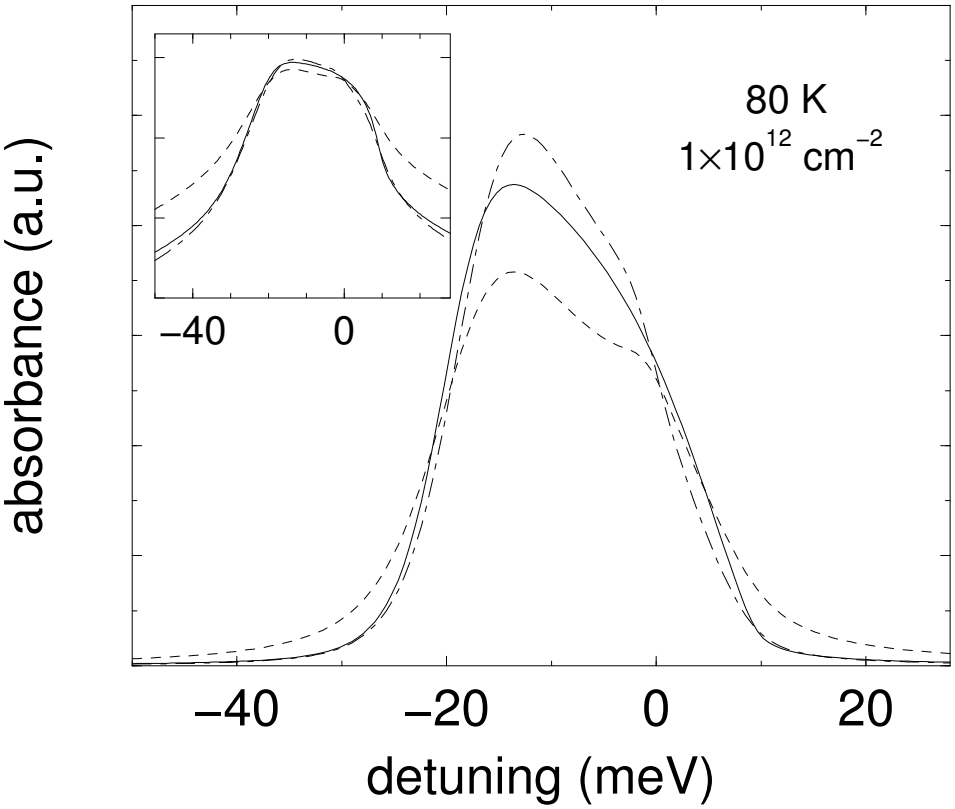

Fig. 3. Intersubband absorption spectra for a 10nm InAs/AlSb quantum well calculated with a constant dephasing rate of 1 mev (solid line), with diagonal scattering term only (dashed line) and with both diagonal and non-diagonal terms (dot-dashed line). The inset shows the same curves but on a Log-scale to show the lineshape differences in the tails.

4 Summary

In summary, we have studied the effects of the interplay of the two collective excitations in intersubband transitions in InAs/AlSb quantum wells and the spectral change as a result of such an interplay. We found that such interplay is critically important in predicting the intersubband lineshape. Depending on the electron density and well width, the lineshape could be dominated by one of the two excitations. Finally, we show that a more complete lineshape treatment including the full second order Coulomb scattering terms, changes the spectral features quantitatively. However, the qualitative features due to the collective excitations remain. Therefore, for a quantitative modeling of the intersubband lineshape, such a more complete treatment of lineshape is necessary.

References

[1] This report has been adapted from work submitted by the same authors to a peer-reviewed journal Physica E: Low-dimensional Systems and Nanostructures.

[2] A. Pinczuk et al, Phys. Rev. Lett. 63 (1989) 1633.

[3] M. Załużny, Phys. Rev. B 43 (1991) 4511.

[4] S. L. Chuang et al, Phys. Rev. B 46 (1992) 1897.

[5] D. Gammon et al., Phys. Rev. Lett. 68 (1992) 1884.

[6] M. S.-C. Luo et al., Phys. Rev. B 48 (1993) 11086.

[7] G. Gumbs, D. Huang, and J. P. Loehr, Phys. Rev. B 51 (1995) 4321.

[8] D. Huang, G. Gumbs and M. O. Manasreh, Phys. Rev. B 52 (1995) 14126.

[9] R. J. Warburton et al., Phys. Rev. B 53 (1996) 7903.

[10] D. E. Nikonov et al., Phys. Rev. Lett. 79 (1997) 4633.

[11] R. J. Warburton et al., Phys. Rev. Lett. 80 (1998) 2185.

[12] B. Nottelmann, V.M. Axt, and T. Kuhn, Physica B 272 (1999) 234.

[13] S. Tsujino et al., Phys. Rev. B 62 (2000) 1560.

[14] J. B. Williams et al., Phys. Rev. Lett. 87 (2001) 037401.

[15] C. A. Ullrich and G. Vignale, Phys. Rev. Lett. 87 (2001) 037402.

[16] J. Li et al., in Progress in Semiconductors II: Electronic and Optoelectronic Applications, B.D. Weaver et al., Eds., MRS (2003) 751.

[17] T. Ando, A. B. Fowler and F. Stern, Rev. Mod. Phys. 54 (1982) 437.

[18] J. Li and C. Z. Ning, Phys. Rev. Lett. 91 (2003) 097401.

[19] W. W. Chow and S. W. Koch, Semiconductor-Laser Fundamentals, Springer-Verlag, Berlin-Heidelberg, 1999.

[20] C.Z. Ning et al., SPIE-Proceedings, 2994 (1997) 666.

[21] T. Kuhn, in Theory of Transport Properties of Semiconductor Nanostructures, E. Schöll, ed., Chapman & Hall, London, 1998, p.173-214.

[22] F. Rossi, S. Haas, and T. Kuhn, Phys. Rev. Lett. 72 (1994) 152.